

Showcasing research from Prof. Wei-Ming Sun's group, School of Pharmacy, Fujian Medical University, Fuzhou, China.

A theoretical study on doping Pd-like superatoms into defective graphene quantum dots: an efficient strategy to design single superatom catalysts for the Suzuki reaction

NbN@GQD, a novel graphene quantum dot (GQD)-supported single superatom catalyst was designed and investigated and exhibits excellent stability and satisfactory catalytic activity for Suzuki reaction. Increasing the number of $-NO_2$ groups at the edge of GQD leads to a progressive improvement in catalytic activity; the fully substituted NbN@GQD-(NO₂)₁₆ catalyst achieves performance comparable to that of Pd@GQD catalyst, providing efficient means to achieving promising alternatives to traditional Pd-based SACs for C–C coupling reactions based on the superatom concept.

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